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                "Ask CAS" for self-help around the clock
                New pricing for the Save Answers for SciFinder Wizard within
NEWS 3 SEP 01
                STN Express with Discover!
NEWS 4 OCT 28
                KOREAPAT now available on STN
NEWS 5 NOV 30 PHAR reloaded with additional data
NEWS 6 DEC 01 LISA now available on STN
                12 databases to be removed from STN on December 31, 2004
NEWS
     7 DEC 09
NEWS
    8 DEC 15
                MEDLINE update schedule for December 2004
NEWS
     9 DEC 17
                ELCOM reloaded; updating to resume; current-awareness
                alerts (SDIs) affected
NEWS 10 DEC 17
                COMPUAB reloaded; updating to resume; current-awareness
                alerts (SDIs) affected
NEWS 11 DEC 17
                SOLIDSTATE reloaded; updating to resume; current-awareness
                alerts (SDIs) affected
                CERAB reloaded; updating to resume; current-awareness
NEWS 12 DEC 17
                alerts (SDIs) affected
NEWS 13 DEC 17
                THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS 14 DEC 30 EPFULL: New patent full text database to be available on STN
NEWS 15 DEC 30
                CAPLUS - PATENT COVERAGE EXPANDED
NEWS 16 JAN 03 No connect-hour charges in EPFULL during January and
                February 2005
NEWS 17 JAN 26
                CA/CAPLUS - Expanded patent coverage to include the Russian
                Agency for Patents and Trademarks (ROSPATENT)
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NEWS EXPRESS JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005

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NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)
```

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Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

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SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 6 FEB 2005 HIGHEST RN 826990-02-7 DICTIONARY FILE UPDATES: 6 FEB 2005 HIGHEST RN 826990-02-7

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10608949d.str

$$G_2$$
 G_1

chain nodes : 11 12 13 15 ring nodes : 1 2 3 4 5 6 7 8 9 chain bonds : 1-11 4-12 12-13 12-15 ring bonds : 1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9 exact/norm bonds : 1-11 5-6 6-7 12-13 12-15 exact bonds : 4-12 5-9 8-9 normalized bonds : 1-2 1-7 2-3 3-4 4-8 7-8 isolated ring systems : containing 1 :

G1:X,Cy,Ak

G2:0,N

Match level :

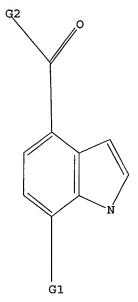
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 11:CLASS 12:CLASS 13:CLASS 15:CLASS

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 X, Cy, Ak G2 O, N

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 08:46:48 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 2757 TO ITERATE

36.3% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

7 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

51991 TO 58289

PROJECTED ANSWERS:

122 TO 648

L2

7 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 08:46:55 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 56148 TO ITERATE

100.0% PROCESSED 56148 ITERATIONS SEARCH TIME: 00.00.03

255 ANSWERS

L3255 SEA SSS FUL L1

=> FIL CAPLUS

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 161.33 161.54

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 08:47:04 ON 07 FEB 2005

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FILE COVERS 1907 - 7 Feb 2005 VOL 142 ISS 7 FILE LAST UPDATED: 6 Feb 2005 (20050206/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s 13
L4
=> s 14 and py<=2002
      22588576 PY<=2002
L5
            20 L4 AND PY<=2002
=> d scan
L5
                   CAPLUS COPYRIGHT 2005 ACS on STN
     37 (Heterocyclic Compounds (One Hetero Atom))
CC
TI
     Structure of melanins and melanogenesis. III. Structure of sepiomelanin
IT
     Spectra, infrared
        (of 3- and 5-methyl pyrrole-2,3,5-tricarboxylates)
ΙT
     Sepiomelanoprotein
IT
     Sepiomelanin
        (structure of)
IT
     37174-47-3, Indole, 5,6,7-trimethoxy-
        (derivs.)
     452-86-8, Pyrocatechol, 4-methyl- 634-97-9, Pyrrole-2-carboxylic acid
IT
     931-03-3, Pyrrole-3-carboxylic acid 937-26-8, Pyrrole-2,4-dicarboxylic
            937-27-9, Pyrrole-2,5-dicarboxylic acid 3131-52-0,
     Indole-5,6-diol 4790-08-3, Indole-2-carboxylic acid, 5,6-dihydroxy-
     90800-62-7, Indole-4,7-dicarboxylic acid, 5,6-dihydroxy-
        (from sepiomelanin decomposition)
IT
     39034-33-8, Pyrrole-2,3,5-tricarboxylic acid, 5-methyl ester 53691-54-6,
     Pyrrole-2,3,5-tricarboxylic acid, 3-methyl ester
        (isolation from methylated sepiomelanin)
IT
     58532-21-1, Indole-2,3-dione, 5,6,7-trimethoxy
                                                       90945-69-0,
     Indole-2,3-dione, 5-hydroxy-6,7-dimethoxy- 93187-34-9,
    \Delta 3, \alpha-Indolineacetonitrile, 5,6,7-trimethoxy-2-oxo-
     95704-83-9, Indole-2-carboxylic acid, 5,6-bis(benzyloxy)-, methyl ester
     101813-10-9, [Δ2,2'-Biindoline]-3,3'-dione, 5,5',6,6',7,7'-
    hexamethoxy-
        (preparation of)
```

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> d hit str 'STR' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ----- GI and AB ALL ----- BIB, AB, IND, RE

APPS ----- AI, PRAI

BIB ----- AN, plus Bibliographic Data and PI table (default) CAN ----- List of CA abstract numbers without answer numbers

CBIB ----- AN, plus Compressed Bibliographic Data

DALL ----- ALL, delimited (end of each field identified)

DMAX ----- MAX, delimited for post-processing

FAM ----- AN, PI and PRAI in table, plus Patent Family data

FBIB ----- AN, BIB, plus Patent FAM

IND ----- Indexing data

IPC ----- International Patent Classifications

MAX ----- ALL, plus Patent FAM, RE

PATS ----- PI, SO

SAM ----- CC, SX, TI, ST, IT

SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers; SCAN must be entered on the same line as the DISPLAY,

e.g., D SCAN or DISPLAY SCAN)

STD ----- BIB, IPC, and NCL

IABS ------ ABS, indented with text labels IALL ------ ALL, indented with text labels IBIB ------ BIB, indented with text labels IMAX ------ MAX, indented with text labels ISTD ------ STD, indented with text labels

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations SIBIB ----- IBIB, no citations

HIT ----- Fields containing hit terms

HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)

containing hit terms

HITRN ----- HIT RN and its text modification

HITSTR ----- HIT RN, its text modification, its CA index name, and

its structure diagram

HITSEQ ----- HIT RN, its text modification, its CA index name, its structure diagram, plus NTE and SEQ fields

FHITSTR ---- First HIT RN, its text modification, its CA index name, and

its structure diagram

FHITSEQ ---- First HIT RN, its text modification, its CA index name, its

structure diagram, plus NTE and SEQ fields

KWIC ----- Hit term plus 20 words on either side

OCC ----- Number of occurrence of hit term and field in which it occurs

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07/02/2005

10608949d.trn

FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):end

=> d l5 ibib abs hitstr tot

L5 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:861062 CAPLUS

DOCUMENT NUMBER: 139:197300

TITLE: Product class 13: indole and its derivatives

AUTHOR(S): Joule, J. A.

CORPORATE SOURCE: Department of Chemistry, University of Manchester,

Manchester, M13 9PL, UK

SOURCE: Science of Synthesis (2001), 10, 361-652

CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review of preparation of indoles and its derivs. Covered reactions include cyclization, ring transformation, aromatization and substituent

modifications. Subclasses covered include 1H-indol-1-ols, 1,3-dihydro-2H-indol-2-ones, and 1,2-dihydro-3H-indol-3-ones.

IT 36800-67-6P 74809-27-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(review of preparation of indoles and analogs thereof via cyclization, ring transformation, aromatization and substituent modifications)

RN 36800-67-6 CAPLUS

CN 1H-Indole-2,4-dicarboxylic acid, 3-(2-carboxyethyl)-7-chloro- (9CI) (CA INDEX NAME)

RN 74809-27-1 CAPLUS

CN 1H-Indole-4,7-dicarboxylic acid, 1-(1,1-dimethylethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

1348 THERE ARE 1348 CITED REFERENCES AVAILABLE FOR

THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L5 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:58 CAPLUS

DOCUMENT NUMBER: 128:57082

TITLE: Discovery and Evaluation of a Series of 3-Acylindole

Imidazopyridine Platelet-Activating Factor Antagonists

AUTHOR(S): Curtin, Michael L.; Davidsen, Steven K.; Heyman, H.

Robin; Garland, Robert B.; Sheppard, George S.; Florjancic, Alan S.; Xu, Lianhong; Carrera, George M., Jr.; Steinman, Douglas H.; Trautmann, Jeff A.; Albert, Daniel H.; Magoc, Terrance J.; Tapang, Paul; Rhein, David A.; Conway, Richard G.; Luo, Gongjin; Denissen, Jon F.; Marsh, Kennan C.; Morgan, Douglas

W.; Summers, James B.

CORPORATE SOURCE: Immunosciences Research Area, Pharmaceutical Products

Division, Abbott Laboratories, Abbott Park, IL,

60064-3500, USA

SOURCE: Journal of Medicinal Chemistry (1998),

41(1), 74-95

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB Studies conducted with the goal of discovering a second-generation platelet-activating factor (PAF) antagonist have identified a novel class

of potent and orally active antagonists which have high aqueous solubility and long

long

duration of action in animal models. The compds. arose from the combination of the lipophilic indole portion of Abbott's first-generation PAF antagonist ABT-299 with the methylimidazopyridine heterocycle moiety of British Biotechnol.'s BB-882 and possess the pos. attributes of both of these clin. candidates. Structure-activity relationship (SAR) studies indicated that modification of the indole and benzoyl spacer of lead compound 1-(N,N-Dimethylcarbamoyl)-6-(4-fluorophenyl)-3-{4-[(1H-2-methylimidazo[4,5-c]pyrid-1-yl)methyl]benzoyl}indole gave analogs that were more potent, longer-lived, and bioavailable and resulted in the identification of 1-(N,N-dimethylcarbamoyl)-4-ethynyl-3-{3-fluoro-4-[(1H-2-methylimidazo[4,5-c]pyrid-1-yl)methyl]benzoyl}indole hydrochloride (ABT-491) which has been evaluated extensively and is currently in clin. development.

IT 170498-16-5P

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(acylindole imidazopyridine PAF antagonist preparation and evaluation)

RN 170498-16-5 CAPLUS

CN 1H-Indole-4,7-dicarboxylic acid, 3-[4-[(2-methyl-1H-imidazo[4,5-c]pyridin-1-yl)methyl]benzoyl]-, dimethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} N \\ N \\ N \\ N \\ CH_2 \\ \end{array}$$

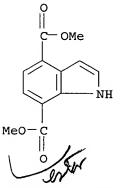
IT 170499-96-4, 4,7-Bis (methoxycarbonyl) indole

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction; acylindole imidazopyridine PAF antagonist preparation and evaluation)

RN 170499-96-4 CAPLUS

CN 1H-Indole-4,7-dicarboxylic acid, dimethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1997:805722 CAPLUS

DOCUMENT NUMBER:

128:34682

TITLE:

Preparation of indole derivatives as cell protective

agents

INVENTOR(S):

Yamamoto, Ichiro; Itoh, Manabu; Shimojo, Masato;

Yumiya, Yasunobu; Mukaihira, Takafumi; Akada,

Yasushige

PATENT ASSIGNEE(S):

Mochida Pharmaceutical Co., Ltd., Japan

PCT Int. Appl., 219 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

SOURCE:

Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9745410 W: CA, JP, KR	A1 , US	19971204	WO 1997-JP1828	19970529 <

	RW: AT,	BE,	CH,	DE,	DK,	ES,	FI,	FR,	GB	GR,	IE,	IT,	LU,	MC.	NL,	PT,	SE
TW	430660			В		2001				1997-					9970		
CA	2228268			AA		1997	1204		CA :	1997-	2228	268		-	19970	529	<
EP	858996			A1		1998	0819		EP :	1997-	9242	54		:	9970	529	<
EP	858996			B1		2004	1027										
	R: AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
	IE,	FΙ															
AT	280758			E		2004	1115	,	AT I	L997-	9242	54		1	9970	529	
	6040331			Α		2000	0321	•	US I	L998-	1126	0			9980	130	< - -
PRIORITY	Y APPLN.	INFO.	. :						JP 1	L996-	1589	85		A :	9960	530	
								1	JP I	1996-	3327	64		A 1	9961	128	
								,	WO 1	L997-	JP18:	28		W 1	9970	529	
OTHER SO	OURCE(S):			MARP	AT	128:	34682	2									

GΙ

$$\mathbb{R}^4$$
 \mathbb{R}^3
 \mathbb{R}^4
 \mathbb{R}^3
 \mathbb{R}^4
 \mathbb{R}^3

AΒ The title compds. (I; R1 = H, CO2H, alkoxycarbonyl, etc.; R2 = halo, C1-4 alkyl or alkoxy, etc.; R3, R4 = H, NR6R7; R5 = H, halo, C1-4 alkyl, etc.; R6, R7 = H, Ph, CHO, alkyl, etc.) are prepared I are useful as analgetic agents and cell protective agents for prevention and treatment of diseases accompanied by the denaturation, retraction or death of nerve cells. Thus, compound (II; X = :0) (preparation given) was treated with NH40Ac and NaBH3CN to give the title compound II (X = NH2), which at 1.0 μ g/mL showed 51% inhibitory activity against death of nerve cells.

IT199664-63-6P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of indole derivs. as cell protective agents)

RN 199664-63-6 CAPLUS

1H-Indole-3-propanoic acid, 4-carboxy-7-chloro-2-phenyl- (9CI) (CA INDEX CN NAME)

ANSWER 4 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 1996:119185 CAPLUS

07/02/2005 10608949d.trn

DOCUMENT NUMBER:

124:317157 TITLE:

Platelet activating factor antagonists:

imidazopyridine indoles

Summers, James B., Jr.; Davidsen, Steven K.; Curtin, Michael L.; Heyman, H. Robin; Sheppard, George S.; Xu, INVENTOR(S):

Lianhong; Carrera, George M., Jr.; Garland, Robert B.

PATENT ASSIGNEE(S): Abbott Laboratories, USA

SOURCE: U.S., 59 pp. Cont.-in-part of U.S. Ser. No. 324,631.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
	A 1996012		
	AA 1995062 A1 1995062		
W: AU, CA, JP,		2 WO 1994-0514112	19941208 <
		, GB, GR, IE, IT, LU,	MC. NL. PT. SE
		3 AU 1995-13036	
AU 690620	B2 1998043	0	
EP 734386	A1 1996100	2 EP 1995-904287	19941208 <
	B1 2002020	-	
		, GB, GR, IE, IT, LI,	
AT 212992		5 AT 1995-904287	
		1 PT 1995-904287	
ES 2173171	T3 2002101		19941208 <
PRIORITY APPLN. INFO.:		US 1993-168564	
		US 1994-324631	
		US 1994-347528	
OFFICE COLUMNIA (A)	MARRAM 404 65-	WO 1994-US14112	W 19941208
OTHER SOURCE(S): GI	MARPAT 124:317	157	

The present invention relates to compds. of formula I wherein: R1 = one or AB more of the groups independently selected from, e.g., H, halo, OH, cyano; R2 is selected from the group consisting of, e.g., H, alkyl of one to 6 C atoms; R3 is selected from the group consisting of H and alkyl of one to six C atoms; L1 = e.g., CO, COCH2NR4 where R4 = e.g., H, alkyl of one to six C atoms; Ar1 is radical II where Y is O, S, or CH:CH, Z is N or CH, R11 = e.g., H, alkyl of one to six C atoms; L2 is selected from, e.g., a valence bond, (un) substituted straight-chain alkylene of one to six C atoms; Ar2 is selected from, e.g., substituted benzimidazol-1-yl, imidazopyridine group III where R13 = e.g., alkyl of one to six C atoms, alkenyl of two to six C atoms; R14 and R15 are independently selected from, e.g., H, alkyl of one to six C atoms, alkenyl of two to six C atoms; and the pharmaceutically acceptable salts thereof which are potent antagonists of PAF and are useful in the treatment of PAF-related disorders including asthma, shock, respiratory distress syndrome, acute inflammation, transplanted organ rejection, gastrointestinal ulceration, allergic skin diseases, delayed cellular immunity, parturition, fetal lung maturation, and cellular differentiation. Thus, e.g., carbamoylation of 6-(4-fluorophenyl)-3-{4-[(1H-2-methylbenzimidazolyl)methyl]benzoyl}indole (preparation given) with dimethylcarbamoyl chloride afforded 1-N, N-dimethylcarbamoyl-6-(4-fluorophenyl)-3-{4-[(1H-2methylbenzimidazolyl)methyl]benzoyl}indole (IV) which exhibited Ki = 56 nM for inhibition of specific [3H]C18-PAF binding.

IT170498-16-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(imidazopyridine indoles as platelet activating factor antagonists)

RN 170498-16-5 CAPLUS

1H-Indole-4,7-dicarboxylic acid, 3-[4-[(2-methyl-1H-imidazo[4,5-c]pyridin-CN 1-yl)methyl]benzoyl]-, dimethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & Me & CH_2 \\ \hline & N & CH_2 \\ \hline & MeO-C \\ \hline & O \\ \hline & MeO-C \\ \hline & O \\ \hline \end{array}$$

IT 170499-96-4P, 4,7-Bis(methoxycarbonyl)indole 175675-75-9P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (imidazopyridine indoles as platelet activating factor antagonists) RN170499-96-4 CAPLUS CN

1H-Indole-4,7-dicarboxylic acid, dimethyl ester (9CI) (CA INDEX NAME)

OMe NН MeO-

RN 175675-75-9 CAPLUS CN 1H-Indole-4,7-dicarboxylic acid, 3-(chloromethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

ANSWER 5 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 1996:104544 CAPLUS

07/02/2005

10608949d.trn

DOCUMENT NUMBER:

124:260071

TITLE:

Theoretical study of the reactions of

1-methyl-2-vinylpyrrole with methyl propiolate and

with dimethyl acetylenedicarboxylate

AUTHOR (S):

Domingo, Luis R.; Jones, R. Alan; Picher, M. Teresa;

Sepulveda-Arques, Jose

CORPORATE SOURCE:

Departament de Quimica Organica, Universitat de Valencia, Dr Moliner 50, 46100-Burjassot, Valencia,

Spain

SOURCE:

THEOCHEM (1996), 362(2), 209-13 CODEN: THEODJ; ISSN: 0166-1280

PUBLISHER: DOCUMENT TYPE:

Elsevier Journal English

LANGUAGE: English

AB A theor. study of the transition structures for the reactions of 1-methyl-2-vinylpyrrole 1 with Me propiolate (MP) and with di-Me acetylenedicarboxylate (DMAD) indicates that, for this vinyl system, the factor controlling the different courses of the reaction is the lower activation energy for the formation of the transition state in the second

cycloaddn. with MP, compared to that with DMAD.

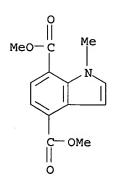
IT 74825-03-9 175400-78-9

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)

(MO study of Diels-Alder reaction 1-methyl-2-vinylpyrrole with Me propiolate and with di-Me acetylenedicarboxylate)

RN 74825-03-9 CAPLUS

CN 1H-Indole-4,7-dicarboxylic acid, 1-methyl-, dimethyl ester (9CI) (CA INDEX NAME)



RN 175400-78-9 CAPLUS

CN 1H-Indole-4,5,6,7-tetracarboxylic acid, 1-methyl-, tetramethyl ester (9CI) (CA INDEX NAME)

ANSWER 6 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:928154 CAPLUS

DOCUMENT NUMBER: 123:340121

TITLE: Preparation of 3-[(imidazopyridylalkyl)benzoyl]indoles

and analogs as platelet activating factor antagonists INVENTOR (S): Summers, James B., Jr.; Davidsen, Steven K.; Curtin, Michael L.; Heyman, H. Robin; Sheppard, George S.; Xu,

Lianhong; Carrera, George M., Jr.; Garland, Robert B.

PATENT ASSIGNEE(S): Abbott Laboratories, USA SOURCE: PCT Int. Appl., 160 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.	KIND DATE	APPLICATION NO.	DATE
	WO 9516687 W: AU, CA, JP,	A1 1995062 KR	2 WO 1994-US14112	19941208 <
	RW: AT, BE, CH,	DE, DK, ES, FR	, GB, GR, IE, IT, LU,	MC, NL, PT, SE
	US 5486525	A 1996012	3 US 1994-347528	19941205 <
	CA 2176247	AA 1995062	2 CA 1994-2176247	19941208 <
	AU 9513036	A1 1995070	3 AU 1995-13036	19941208 <
	AU 690620	B2 1998043	0	
	EP 734386	A1 1996100	2 EP 1995-904287	19941208 <
		B1 2002020		
			, GB, GR, IE, IT, LI,	LU, NL, PT, SE
	AT 212992	E 2002021	5 AT 1995-904287	19941208 <
PRIO	RITY APPLN. INFO.:		US 1993-168564	A 19931216
			US 1994-324631	A 19941018
			US 1994-347528	A 19941205
			WO 1994-US14112	W 19941208
OTHER	R SOURCE(S):	MARPAT 123:340	121	

OTHER SOURCE(S): MARPAT 123:340121

GΙ

Title compds. [I; R = Z1Z2Z3R4; R1 = H, halo, alkyl, alkoxy, etc.; R2 = H, (carboxy)alkyl, aminoalkyl, etc.; R3 = H, alkyl; R4 = (hetero)anellated imidazolyl, etc.; Z1 = CO, CONH, C(:NNH2), etc.; Z2 = bond, phenylene, heteroarylene, etc.; Z3 = bond, (un)substituted alkylene] were prepared Thus, 4-bromoindole was converted in 4 steps to I (R = COC6H4CH2NH2, R1 = 4-Br, R2 = CONMe2, R3 = H) which was N-alkylated by 4-ethoxy-3-nitropyridine and the product converted in 2 steps to title compound II (R1 = Br). The latter was alkylated by Me3SnC.tplbond.CSiMe3 to give, after deprotection, II (R1 = C.tplbond.CH) which had Ki of 0.6nM for platelet activating factor inhibition in vitro.

IT 170498-16-5P

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 3-[(imidazopyridylalkyl)benzoyl]indoles and analogs as platelet activating factor antagonists)

RN 170498-16-5 CAPLUS

1H-Indole-4,7-dicarboxylic acid, 3-[4-[(2-methyl-1H-imidazo[4,5-c]pyridin-1-yl)methyl]benzoyl]-, dimethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & Me \\ \hline N & CH_2 \\ \hline \end{array}$$

IT 170499-57-7P 170499-96-4P, Dimethyl indole-4,7dicarboxylate

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 3-[(imidazopyridylalkyl)benzoyl]indoles and analogs as platelet activating factor antagonists)

RN 170499-57-7 CAPLUS

RN 170499-96-4 CAPLUS

CN 1H-Indole-4,7-dicarboxylic acid, dimethyl ester (9CI) (CA INDEX NAME)

L5 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1995:264059 CAPLUS

DOCUMENT NUMBER:

122:133016

TITLE:

Synthesis of pyrano[4,3-b] azepines by [4+2]

cycloaddition of photochemically generated

3-alkoxycarbonyl-1,2-didehydroazepines with enol

ethers

AUTHOR (S):

Tueckmantel, Werner

CORPORATE SOURCE:

Pharmazeutisch-Chem. Inst., Univ. Heidelberg,

Heidelberg, D-69120, Germany

SOURCE:

LANGUAGE:

Liebigs Annalen der Chemie (1994), (12),

1165-71

CODEN: LACHDL; ISSN: 0170-2041

PUBLISHER: DOCUMENT TYPE:

VCH Journal English

OTHER SOURCE(S):

CASREACT 122:133016

3-Alkoxycarbonyl-1,2-didehydroazepines, generated by photolysis of alkyl 2-azidobenzoates, undergo a hetero-[4 + 2] cycloaddn. (stepwise or concerted) with ketone-derived enol ethers to form intensely colored, paratropic 6,8-dialkoxy-8,9-dihydropyrano[4,3-b]azepines, which contain the unusual 3-azaheptafulvene partial structure. Other derivs. of 2-azidobenzoic acid as well as aldehyde-derived enol ethers, other classes of olefins, phenol ethers, and furans are unreactive although 2-methoxynaphthalene undergoes demethylation to produce Me 2-(2-naphthyloxy)-3H-azepine-3-carboxylate. Acid-catalyzed hydrolysis of

07/02/2005

10608949d.trn

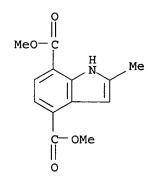
the title compds. produces 2-(acylmethylene)-2,3-dihydro-1H-azepine-3carboxylates and indoles; catalytic hydrogenation generates a tetrahydro derivative, and diastereomeric tricarbonylation complexes are formed with Fe2(CO)9 at the conjugated diene moiety. An intensely colored byproduct of the photolysis reaction is identified as the first known derivative of 3,3'-diazaheptafulvalene.

IT 160777-53-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN160777-53-7 CAPLUS

CN 1H-Indole-4,7-dicarboxylic acid, 2-methyl-, dimethyl ester (9CI) INDEX NAME)



ANSWER 8 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1994:106973 CAPLUS

DOCUMENT NUMBER:

120:106973

TITLE:

Preparation of indoledicarboxymides as antitumor

agents

INVENTOR(S):

Nagai, Takashi; Myokan, Isao; Funaki, Takashi; Nomura,

Yoko; Mizutani, Masatoshi; Hori, Takako

PATENT ASSIGNEE(S):

SOURCE:

Toyama Chemical Co Ltd, Japan Jpn. Kokai Tokkyo Koho, 25 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent Japanese

LANGUAGE: FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05202048	A2	19930810	JP 1992-38615	19920129 <
JP 3178880	B2	20010625		
PRIORITY APPLN. INFO.:			JP 1992-38615	19920129
OTHER SOURCE(S):	MARPAT	120:106973		
GT				

AB The title compds. I [R1 = H, (substituted) alkyl, alkenyl, aryl, etc.; R2 = H, (substituted) alkyl, acyl, etc.; R3 = H, halo, (substituted) alkyl, cycloalkyl, etc.; Y = bond, alkylene; Z = halo, NR4R5, etc.; R4, R5 = H, (substituted) alkyl, cycloalkyl, acyl, etc.; or NR4R5 = (substituted) N-containing heterocyclic ring] were prepared Condensation of 3,7-dimethyl-2-phenylindole-4,5-dicarboxylic acid anhydride with N,N-dimethylethylenediamine in xylene gave N-(2-dimethylaminoethyl)-3,7-dimethyl-2-phenyl-indole-4,5-dicarboxyimide. The title compds. in vitro had MIC values of 1.56-6.25 μg/mL against tumor HeLA S3 cells.

IT 152294-66-1P 152294-67-2P 152294-68-3P 152294-69-4P 152294-70-7P 152294-71-8P 152294-72-9P 152294-78-5P 152294-79-6P

Ι

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of antitumor agent)

RN 152294-66-1 CAPLUS

CN 1H-Indole-4,5-dicarboxylic acid, 3,7-dimethyl-2-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{H} & \text{Ph} \\ \hline & \text{MeO-C} & \text{Me} \\ \hline & \text{O} & \text{C-OMe} \\ \hline & \text{O} & \\ \end{array}$$

RN 152294-67-2 CAPLUS

CN 1H-Indole-4,5-dicarboxylic acid, 2,3,7-trimethyl-, dimethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ MeO-C & & & \\ & & & \\ O & & & \\ & & & \\ O & & & \\ & & & \\ O & & \\ & & & \\ \end{array}$$

RN 152294-68-3 CAPLUS

CN 1H-Indole-4,5-dicarboxylic acid, 2-(4-methoxyphenyl)-3,7-dimethyl-, dimethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & Me \\ & H \\ \hline N \\ O \\ C \\ O \\ C \\ O \\ O \\ \end{array}$$

RN 152294-69-4 CAPLUS

CN lH-Indole-4,5-dicarboxylic acid, 3,7-dimethyl-2-(3,4,5-trimethoxyphenyl)-, dimethyl ester (9CI) (CA INDEX NAME)

RN 152294-70-7 CAPLUS

CN 1H-Indole-4,5-dicarboxylic acid, 3,7-dimethyl-2-(2-naphthalenyl)-, dimethyl ester (9CI) (CA INDEX NAME)

RN 152294-71-8 CAPLUS

CN 1H-Indole-4,5-dicarboxylic acid, 3,7-dimethyl-2-(4-pyridinyl)-, dimethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & Me & H \\ & H \\ N & \\ & N \\ & C - OMe \\ & \\ & O \end{array}$$

RN 152294-72-9 CAPLUS

CN 1H-Indole-4,5-dicarboxylic acid, 3,7-dimethyl-2-(2-thienyl)-, dimethyl ester (9CI) (CA INDEX NAME)

RN 152294-78-5 CAPLUS

CN Pyridinium, 4-[4,5-bis(methoxycarbonyl)-3,7-dimethyl-1H-indol-2-yl]-1-methyl-, iodide (9CI) (CA INDEX NAME)

• I-

RN 152294-79-6 CAPLUS

CN 1H-Indole-4,5-dicarboxylic acid, 3,7-dimethyl-2-(1,2,3,6-tetrahydro-1-methyl-4-pyridinyl)-, dimethyl ester (9CI) (CA INDEX NAME)

L5 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:151256 CAPLUS

DOCUMENT NUMBER: 116:151256

TITLE: Copper(II) in organic synthesis. IX. The

copper(II)-catalyzed Michael reaction as a route to

polysubstituted benzene derivatives

AUTHOR(S): Desimoni, Giovanni; Invernizzi, Anna Gamba; Quadrelli,

Paolo; Righetti, Pier Paolo

CORPORATE SOURCE: Dip. Chim. Org., Univ. Pavia, Pavia, I-27100, Italy

SOURCE: Gazzetta Chimica Italiana (1991), 121(10),

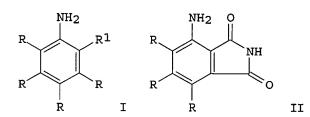
483-5

CODEN: GCITA9; ISSN: 0016-5603

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 116:151256

GΙ



- AB Cyclization of RC.tplbond.CR (R = CO2Me) with R1CH2CN (R1 = CN, CO2Me) in dioxane catalyzed by Cu2(OAc)4, gave 20-41% anilines I, whereas H2NCOCH2CN gave 16% II.
- IT 139286-25-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and spectra of)

RN 139286-25-2 CAPLUS

CN 1H-Indole-2,3,4,5,6,7-hexacarboxylic acid, hexamethyl ester (9CI) (CF INDEX NAME)

L5 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1991:583012 CAPLUS

DOCUMENT NUMBER:

115:183012

TITLE:

[4+2] Cycloaddition reaction of N-(ethoxycarbonyl)-2-

[1-(trimethylsiloxy)vinyl]pyrrole with acetylenic

carboxylates

AUTHOR (S):

Ohno, Masatomi; Shimizu, Sadahiro; Eguchi, Shoji

CORPORATE SOURCE:

Fac. Eng., Nagoya Univ., Nagoya, 464, Japan

Heterocycles (1991), 32(6), 1199-202

SOURCE:

CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 115:183012

GI

$$CO_2Me$$
 CH_2
 EtO_2C
 $OSiMe_3$
 I
 EtO_2C
 OH
 II

AB The title reaction resulted in the formation of functionalized indoles through rearomatization via ene reaction followed by elimination or via competitive air oxidation Under an atmospheric of oxygen the latter process predominated to give majorly 7-hydroxy substituted indoles. Thus, the reactions of the title pyrrole I with RC.tplbond.CCO2Me (R = H, CO2Me) in the presence of air or oxygen gave hydroxyindoles II.

IT 136497-17-1P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN136497-17-1 CAPLUS

CN 1H-Indole-1,4,5-tricarboxylic acid, 7-[3-methoxy-1-(methoxycarbonyl)-3-oxo-1-propenyl]-, 1-ethyl 4,5-dimethyl ester (9CI) (CA INDEX NAME)

L5 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:424169 CAPLUS

DOCUMENT NUMBER: 105:24169

TITLE: Syntheses and properties of 2-amino-3-oxo-3H-azepines

AUTHOR(S): Eicher, Theophil; Kruse, Alfred

CORPORATE SOURCE: Fachber. 14 Org. Chem., Univ. Saarlandes,

Saarbruecken, D-6600/11, Fed. Rep. Ger.

SOURCE: Synthesis (1985), (6-7), 612-19

CODEN: SYNTBF; ISSN: 0039-7881

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 105:24169

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- The aminodibenzazepinones I [R = piperdino, morpholino, NEt2, NCHMe2)2, NHCHMe2, NHPh] were obtained in 45-77% yield by treating 5-tosyl-6,7-dihydro-5H-dibenz[b,d]azepin-7-one with EtO2CCH2CH2P+Ph3 Br3-. The aminobenzazepinones II (R = NEt2, NHCHMe2) were similarly prepared The 3-benzazepin-1-one III was obtained from the 4,5-dihydro derivative by bromination-dehydrobromination. The chemical and spectroscopic properties of I-III are discussed.
- IT 102913-14-4P

RN 102913-14-4 CAPLUS

CN 1H-Indole-4,5,7-tricarboxylic acid, 2,3-dimethyl-, trimethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ \\ MeO-C \\ \\ \hline \\ O \\ \hline \\ O \\ \\ \end{array} \begin{array}{c} H \\ \\ Me \\ \\ \\ \\ \\ O \\ \end{array} \begin{array}{c} Me \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{array}$$

L5 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1985:131299 CAPLUS

DOCUMENT NUMBER: 102:131299

TITLE: Pyrrole studies. Part 28. The effect of steric

hindrance upon the reaction of 2-vinylpyrroles with

dimethyl acetylenedicarboxylate

AUTHOR(S): Jones, R. Alan; Saliente, Teresa Aznar; Arques, Jose

Sepulveda

CORPORATE SOURCE: Sch. Chem. Sci., Univ. East Anglia, Norwich, NR4 7JT,

UK

SOURCE: Journal of the Chemical Society, Perkin Transactions

1: Organic and Bio-Organic Chemistry (1972-1999) (

1984), (11), 2541-3

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 102:131299

GI

$$\mathbb{N}_{\mathbb{R}}$$
 $\mathbb{C}\mathbb{R}^1 = \mathbb{C}\mathbb{H}_2$

AB The reactions of the vinylpyrroles I (R = Me, R1 = H, Me, CMe3, Ph; R = Ph, R1 = H, Me) with MeO2CC.tplbond.CCO2Me (II) in CHCl3 were examined at 20 and 60°. Steric interaction between R and R1 destabilizes the cisoid conformation of I, thereby inhibiting $(\pi 4 + \pi 2)$ -cycloaddn. reactions. Bulky N-substituents also sterically inhibited the Michael addition of II at the 5-position of the ring.

IT 94633-41-7P

RN 94633-41-7 CAPLUS

CN 1H-Indole-4,5-dicarboxylic acid, 7-methyl-1-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)

L5 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1983:452768 CAPLUS

DOCUMENT NUMBER: 99:52768

TITLE: Diels-Alder reactions of vinyl derivatives of

five-membered monoheterocyclic compounds

AUTHOR (S): Noland, Wayland E.; Lee, Chang Kiu; Bae, Sun Kun;

Chung, Bong Yul; Hahn, Chi Sun; Kim, Keun Jae

CORPORATE SOURCE: Sch. Chem., Univ. Minnesota, Minneapolis, MN, 55455,

USA

Journal of Organic Chemistry (1983), 48(15), SOURCE:

2488-91

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE:

English OTHER SOURCE(S): CASREACT 99:52768

Vinylpyrroles having electron-withdrawing substituents react with

dienophiles to give [4 + 2] π adducts while the furan and thiophene analogs do not due to the greater electron-releasing ability of the N atom in the pyrrole. The s-cis conformation of the (1H-pyrrol-2-yl) maleate derivs. is an important factor in their cycloaddn. reaction.

TT

86012-84-2P 86012-89-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN86012-84-2 CAPLUS

CN1H-Indole-4,6,7-tricarboxylic acid, trimethyl ester (9CI) (CA INDEX NAME)

RN86012-89-7 CAPLUS

1H-Indole-4,5,6,7-tetracarboxylic acid, 1-(2,6-dimethylphenyl)-, CNtetramethyl ester (9CI) (CA INDEX NAME)

L5 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1981:425087 CAPLUS

DOCUMENT NUMBER:

95:25087

TITLE:

Indolobenzoxazines
Jones, James H.

INVENTOR(S):
PATENT ASSIGNEE(S):

Merck and Co., Inc., USA

SOURCE:

U.S., 9 pp. CODEN: USXXAM

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT	NO.	KIND	DATE	APPLICATION N	10.	DATE
US 423 EP 337		A A1	19801209 19810819	US 1979-96966 EP 1980-10720		19791123 < 19801120 <
EP 337	67	B1	19840627		, 0	13001120
			FR, GB, IT,	LU, NL, SE		
AT 814	4	E	19840715	AT 1980-10720	16	19801120 <
DK 800	4975	Α	19810524	DK 1980-4975		19801121 <
AU 806	4594	A1	19810528	AU 1980-64594		19801121 <
AU 539	028	B2	19840906			
ES 497	064	A1	19820401	ES 1980-49706	54	19801121 <
ZA 800	7295	A	19820630	ZA 1980-7295		19801121 <
JP 560	87583	A2	19810716	JP 1980-16476	8	19801125 <
JP 020	27358	B4	19900615			
PRIORITY AF				US 1979-96966	A	19791123
				EP 1980-10720	6 A	19801120
CT				== =====		

GI

The indolobenzoxazines I (R = H, alkyl, aryl; R1 = H, alkyl, aralkyl, AB cycloalkyl, alkenyl; R2 = H, halo, alkyl; R3 = H, alkyl, aralkyl; R4 = H, halo, alkyl, hydroxy, alkoxy) were prepared Thus, the benzindole II (R5 = H) was treated with ClCH2COCl to give II (R5 = ClCH2CO), which was cyclized followed by LiAlH4 reduction to give I (R-R4 = H). At 50-500 mg/kg I were antihypertensive, and at 20-100 mg/kg had antiparkinson and prolactin-inhibiting activity.

TT 36800-76-7

> RL: RCT (Reactant); RACT (Reactant or reagent) (cyclization of)

RN 36800-76-7 CAPLUS

CN 1H-Indole-3-propanoic acid, 4-carboxy-7-chloro- (9CI) (CA INDEX NAME)

CAPLUS COPYRIGHT 2005 ACS on STN ANSWER 15 OF 20

ACCESSION NUMBER: 1981:3909 CAPLUS

DOCUMENT NUMBER: 94:3909

TITLE: Electrophilic reactions of dimethyl

> acetylenedicarboxylate with a cyclic dienamine: solvent influence upon the competitive formation of

[4+2]-, [2+2]- and Michael type adducts

AUTHOR (S): Eberbach, Wolfgang; Carre, Jean Claude

CORPORATE SOURCE: Chem. Lab., Univ. Freiburg, Freiburg, D-7800, Fed.

Rep. Ger.

SOURCE: Tetrahedron Letters (1980), 21(12), 1145-8

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 94:3909

GI

CH₂Ph
$$\frac{\text{MeO}_2\text{C}}{\text{NCH}_2\text{Ph}}$$
 $\frac{\text{NCH}_2\text{Ph}}{\text{CO}_2\text{Me}}$ $\frac{\text{CO}_2\text{Me}}{\text{I}}$ $\frac{\text{MeO}_2\text{C}}{\text{CO}_2\text{Me}}$ $\frac{\text{NCH}_2\text{Ph}}{\text{CO}_2\text{Me}}$

The azepine I (R = H) reacted with MeO2CC.tplbond:CCO2Me in CCl4, MeCN, and MeOH to give the adducts II, III, and I [R = (E)-MeO2CCH:C(CO2Me)], resp. The mechanism and effect of solvent are discussed.

IT 75817-91-3P

RN 75817-91-3 CAPLUS

CN 1H-Indole-2,4,6,7-tetracarboxylic acid, 1-(phenylmethyl)-, tetramethyl ester (9CI) (CA INDEX NAME)

L5 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1980:639132 CAPLUS

DOCUMENT NUMBER:

93:239132

TITLE:

Pyrrole studies. 22. $[4\pi + 2\pi]$ Cycloaddition

reactions with vinylpyrroles

AUTHOR(S):

Jones, R. Alan; Marriott, Michael T. P.; Rosenthal, W.

Philip; Sepulveda Arques, Jose

CORPORATE SOURCE:

Sch. Chem. Sci., Univ. East Anglia, Norwich/Norfolk,

NR4 7TJ, UK

SOURCE:

Journal of Organic Chemistry (1980), 45(22),

07/02/2005

10608949d.trn

4515-19

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE:

Journal English

LANGUAGE: OTHER SOURCE(S):

CASREACT 93:239132

GI

Diels-Alder reaction of 2- and 3-vinylpyrroles with electron-deficient dienophiles gave 4 dihydro- and 9 tetrahydroindoles, which underwent sigmatropic H migration leading to aromatization of the 5-membered ring. Thus, cycloaddn. of 1-methyl-2-vinylpyrrole with MeO2CC.tplbond.CCO2Me gave 67% di-Me 1-methyl-6,7-dihydroindole-4,5-dicarboxylate, which was aromatized by refluxing with 2,3-dichloro-5,6-dicyanoquinone in dry C6H6 0.5 h to give 25% di-Me 1-methylindole-4,5-dicarboxylate (I). Among the 7 other indoles similarly prepared were di-Me 1-phenylindole-4,7-dicarboxylate and Me 1-tert-butylindole-7-carboxylate.

IT 74809-24-8P 74809-27-1P 74825-03-9P

RN 74809-24-8 CAPLUS

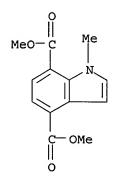
CN 1H-Indole-4,7-dicarboxylic acid, 1-phenyl-, dimethyl ester (9CI) (CA INDEX NAME)

RN 74809-27-1 CAPLUS

CN 1H-Indole-4,7-dicarboxylic acid, 1-(1,1-dimethylethyl)-, dimethyl ester (9CI) (CA INDEX NAME)

RN 74825-03-9 CAPLUS

CN 1H-Indole-4,7-dicarboxylic acid, 1-methyl-, dimethyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1980:586626 CAPLUS

DOCUMENT NUMBER: 93:186626

TITLE: Preparative methods for ergoline synthons: Uhle's

ketone and the C-homo analog

AUTHOR(S): Ponticello, G. S.; Baldwin, J. J.; Lumma, P. K.;

McClure, D. E.

CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., Dep. Med. Chem., West

Point, PA, 19486, USA

SOURCE: Journal of Organic Chemistry (1980), 45(21),

4236-8

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

AB Preparative methods are described for the synthesis of the tricyclic indolo ketones I (n = 1, 2); these compds. are useful intermediates for the construction of ergolines and related ring systems. The synthetic strategy involves a Dieckmann cyclization-decarboxylation sequence from the diesters II (n = 2,3).

36800-68-7P 74724-99-5P IT

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and dechlorination of)

RN 36800-68-7 CAPLUS

CN 1H-Indole-2,4-dicarboxylic acid, 3-(2-carboxyethyl)-7-chloro-, 2-ethyl ester (9CI) (CA INDEX NAME)

RN74724-99-5 CAPLUS

CN1H-Indole-2,4-dicarboxylic acid, 3-(3-carboxypropyl)-7-chloro-, 2-ethyl ester (9CI) (CA INDEX NAME)

ANSWER 18 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1972:405270 CAPLUS

DOCUMENT NUMBER: 77:5270

TITLE: 1,3,4,5-Tetrahydrobenz[c,d]indoles and related

compounds. I. New synthesis of 3,4-

dihydrobenz[c,d]indol-5(1H)-one (Uhle's ketone)

AUTHOR (S): Bowman, R. E.; Goodburn, T. G.; Reynolds, A. A.

CORPORATE SOURCE: Res. Dev. Div., Parke Davis and Co., Pontypool, UK SOURCE: Journal of the Chemical Society, Perkin Transactions

1: Organic and Bio-Organic Chemistry (1972-1999) (

1972), (9-10), 1121-3

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 77:5270 GI For diagram(s), see printed CA Issue.

-Carboxy-2-chlorobenzenediazonium chloride reacted with Et AB

2-oxocyclopentanecarboxylate followed by hydrolysis to give 1-Et H

2-oxohexanedioate (5-carboxy-2-chlorophenyl)hydrazone (I). Treatment of I

with BF3.AcOH in AcOH at 90° gave 81% 4-carboxy-7-chloro-2- (ethoxycarbonyl)indole-3-propionic acid, which was converted in 67% overall yield to 4-carboxyindole-3-propionic acid (II) by sequential hydrolysis, hydrogenolysis, and thermal decarboxylation. II was readily converted to Uhle's ketone (III) by standard methods.

IT 36800-67-6P 36800-68-7P 36800-76-7P

36800-77-8P

RN 36800-67-6 CAPLUS

CN 1H-Indole-2,4-dicarboxylic acid, 3-(2-carboxyethyl)-7-chloro- (9CI) (CA INDEX NAME)

$$C1$$
 H
 CO_2H
 $CH_2-CH_2-CO_2H$
 CO_2H

RN 36800-68-7 CAPLUS

CN 1H-Indole-2,4-dicarboxylic acid, 3-(2-carboxyethyl)-7-chloro-, 2-ethyl ester (9CI) (CA INDEX NAME)

RN 36800-76-7 CAPLUS

CN 1H-Indole-3-propanoic acid, 4-carboxy-7-chloro- (9CI) (CA INDEX NAME)

RN 36800-77-8 CAPLUS

CN 1H-Indole-3-propanoic acid, 7-chloro-4-(ethoxycarbonyl)-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 & H & O \\ \hline & H & N & O \\ \hline & CH_2-CH_2-C-OEt \\ \hline & O & \\ \hline & O & \\ \end{array}$$

ANSWER 19 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1964:38666 CAPLUS

DOCUMENT NUMBER: 60:38666 ORIGINAL REFERENCE NO.: 60:6810b-q

TITLE: Structure of melanins and melanogenesis. III.

Structure of sepiomelanin

AUTHOR (S): Piattelli, M.; Fattorusso, E.; Magno, S.; Nicolaus, R.

CORPORATE SOURCE: Univ. Naples

SOURCE: Tetrahedron (1963), 19(12), 2061-72

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

Sepiomelanin (I) on alkali fusion gave cf. CA 57, 16532f. 5,6-dihydroxyindole (II), 4-methylpyrocatechol (III), 5,6-dihydroxyindole-2-carboxylic acid (IV), pyrrole-2-carboxylic acid (V), pyrrole-3-carboxylic acid (VI), pyrrole-2,4-dicarboxylic acid (VII), pyrrole-2,5-dicarboxylic acid (VIII), and 5,6-dihydroxyindole-4,7dicarboxylic acid. Similar alkaline fusion of 5,6-dihydroxyindolemelanin gave II, pyrocatechol, V, VI, VII, and VIII. Analogous treatment of 2,2'-dihydroxybiphenyl gave o-HOC6H4CO2H, PhOH, and o-MeC6H4OH. ml.) containing 3 g. 5,6-bis(benzyloxy)indole-2-carboxylic acid (IX) hydrogenated at 95°/100 atmospheric 48 hrs. with 400 mg. 10% Pd-C gave 1.6 g. IV, m. 230° (dilute AcOH). Methylated I(30 g.) oxidized with H2O2 in AcOH gave 5-carbomethoxypyrrole-2,3-dicarboxylic acid (X), m. 246-7°, 3-carbomethoxypyrrole-2,5-dicarboxylic acid (XI), m. 249-51° (H2O), and H2C(CO2H)2, m. 135-6°, by different isolation techniques. The isolation of XI further proved that indole units with a CO2H group in position 2 are present in I. The presence of these units shows that a carboxylated intermediate, probably dopachrome, partakes in the formation of the polymer. Whether these units retain an aminochrome structure in the polymer or rearrange to units of dihydroxyindole type was determined by preparation of a melanin by enzymic oxidation of

IV with tyrosinase to give melanin(XII). XII (50 mg.) oxidized 10 days at 20° with 3.0 ml. 1:1 AcOH 36% H2O2 gave pyrrole-2,3,5-tricarboxylic acid (XIII), pyrrole-2,3,4,5-tetracarboxylic acid (XIV), glycine, and aspartic acid. IX (1 g.) in Et20 treated with CH2N2 in Et20 gave 2-carbomethoxy-5,6-bis-(benzyloxy) indole, m. 149-50°, which was hydrogenated to 2-carbomethoxy-5,6-dihydroxyindole (XV), m. 255-60°. XV (550 mg.) in 10 ml. 2N K2CO3 oxidized with 60 ml. 3% aqueous KMnO4 gave 30 mg. X, m. 246-7°. A suspension of 100 mg. 2,3,5-tricarbomethoxypyrrole in 9 ml. 0.1N NaOH kept 14 hrs. and the clear solution acidified with concentrated HCl gave 25 mg. XI, m. 249-51° (H2O), giving a red color with diazotized p-H2NC6H4SO3H. XII (248 mg.), dried at 80° over P2O5 in vacuo 8 hrs., was decarboxylated according to P.

and N. (CA 55, 11433h) to give 64 mg. BaCO3, equivalent to 5.9% XII. The decarboxylated XII (50 mg.) oxidized with 3% aqueous KMnO4 gave XIII and XIV. Titration of the CO2H groups of XII gave a neutralization equivalent 180 [theoretical for (C9H3NO4)x 189]. Since it has been shown that the CO2H groups at position 2 and those derived from partial degradation of some indole nuclei during melanogenesis are eliminated by heating I, it was assumed that in the natural pigment the carboxylated units have a dopachrome structure. I oxidized with H2O2AcOH gave cysteic acid, taurine, aspartic acid, and glycine. The presence of cysteic acid shows that the bond between the prosthetic part and the protein in sepiomelanoprotein is effected by the intervention of the SH groups of cysteine mols. Taurine is probably an artifact originating by decarboxylation of cysteine residues. Aspartic acid and glycine may be derived from the nonprotein moiety of the pigment since they also were obtained by H2O2-AcOH oxidation of IV.

IT 90800-62-7, Indole-4,7-dicarboxylic acid, 5,6-dihydroxy-(from sepiomelanin decomposition)

RN 90800-62-7 CAPLUS

CN Indole-4,7-dicarboxylic acid, 5,6-dihydroxy- (7CI) (CA INDEX NAME)

L5 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1963:59659 CAPLUS

DOCUMENT NUMBER:
ORIGINAL REFERENCE NO.:

58:59659 58:10167d-f

TITLE:

Addition reactions of heterocyclic compounds. XIV. The

pyrolysis and hydrolysis of tetramethyl

3a,7a-dihydro-1-methylindole-2,3,3a,4-tetracarboxylate

AUTHOR(S): Acheson, R. M.; Vernon, J. M.

CORPORATE SOURCE:

Univ. Oxford, UK

SOURCE:

Journal of the Chemical Society, Abstracts (

1963) 1907-13

CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE:

Journal

LANGUAGE:

Unavailable

GI For diagram(s), see printed CA Issue.

AB Pyrolysis of III with Pd-C gave trimethyl 1-methylindole-2,3,4-tricarboxylate (IV) and V, the latter through a 1,2-shift of the angular ester group; pyrolysis in Ph2O gave tetramethyl 1-methylindole-2,3,6,7-tetracarboxylate and trimethyl 1-methylpyrrole-2,3,4-tricarboxylate. Alkaline hydrolysis of III and treatment with CH2N2 gave trimethyl 6,7-dihydro-1-methylindole-2,3,4-tricarboxylate which was oxidized to (IV) and with dimethyl acetylenedicarboxylate gave a mixture of 1-methylindoletetra- and pentacarboxylic esters.

IT 95428-37-8, Indole-2,3,4,6,7-pentacarboxylic acid, 1-methyl-,
 pentamethyl ester

(preparation of)

RN 95428-37-8 CAPLUS

CN Indole-2,3,4,6,7-pentacarboxylic acid, 1-methyl-, pentamethyl ester (7CI)

(CA INDEX NAME)

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